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Dr. Richard S. Miller
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6. AUTHOR(S)
Peter Politzer, J. S. Murray and M. E. Grice

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of New Orleans
Department of Chemistry
New Orleans, Louisiana 70148

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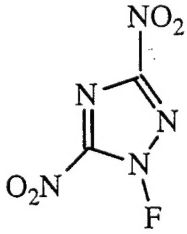
The predicted heat of formation and impact sensitivity of the recently-synthesized dinitro-N-fluorotriazole **1**,



1

based on computational analyses, are:

ΔH_f (gaseous) = 77 kcal/mole = 435 cal/gram

ΔH_f (solid) = 56 kcal/mole = 316 cal/gram

h_{50} = 126 cm

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Dr. Richard S. Miller

Technical Report No. 90

COMPUTED HEAT OF FORMATION AND IMPACT SENSITIVITY OF A NEW DINITRO-N-FLUOROTRIAZOLE

by

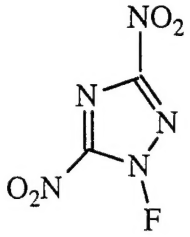
Peter Politzer, J. S. Murray and M. E. Grice

Department of Chemistry
University of New Orleans
New Orleans, LA 70148

March 7, 1996

The dinitro-N-fluorotriazole **1** has recently been synthesized [1] and characterized crystallographically [2].

1



We now report our computed heat of formation and impact sensitivity for **1**.

The gas phase heat of formation was calculated using our density functional procedure [3]. It was converted to the solid phase value by means of eq. (1),

$$\Delta H_f\,(\text{solid}) = \Delta H_f\,(\text{gaseous}) - \Delta H_{sub} \qquad (1)$$

in which ΔH_{sub} is the heat of sublimation. ΔH_{sub} and the impact sensitivity, h_{50}, were obtained by means of correlations that we have developed between these properties and computed quantities related to electrostatic potentials on molecular surfaces [4,5]. The latter were calculated at the *ab initio* HF/STO-5G//HF/3-21G level.

The results follow:

$\Delta H_f\,(\text{gaseous}) = 77$ kcal/mole = 435 cal/gram

$\Delta H_f\,(\text{solid}) = 56$ kcal/mole = 316 cal/gram

$h_{50} = 126$ cm

References

[1] R. J. Schmitt, SRI International.

[2] R. Gilardi, Naval Research Laboratory.

[3] D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and Peter Politzer, J. Comp. Chem. 16, 654 (1995).

[4] ΔH_{sub}: E. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.

[5] h_{50}: J. S. Murray, P. Lane and P. Politzer, Mol. Phys. 85, 1 (1995).